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EXCHANGE SCATTERING IN A THREE-BODY PROBLEM

by

HARRY E. MOSES

CONTRACT No. AF-19(122)-463

CX-5 c.1

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The research reported in this document has been made possible through support and sponsorship extended by the Geophysics Research Division of the Air Force Cambridge Research Center, under Contract No. AF-19(122)-463. It is published for technical information only, and does not necessarily represent recommendations or conclusions of the sponsoring agency.

January 1953

Manufactured in the United States of America by the
Office of Publications and Printing of
New York University

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Abstract

It is proved that in the three-body scattering problem, the prototype of which is the scattering of an electron by a hydrogen atom, the coefficient corresponding to exchange scattering behaves like a radially outgoing wave. The essential conjecture used by Mott and Massey (Ref. 1) in their treatment of the problem is thus verified.

1. Introduction

We shall consider the problem of the scattering of an electron by a hydrogen atom the nucleus of which is considered to be infinitely heavy. We shall take the case where the electrons are considered identifiable. Furthermore, since we do not wish to discuss convergence difficulties arising from the fact that Coulomb forces die out slowly, we shall replace the Coulomb interactions by shorter-range interactions.

Mott and Massey (ref. 1) treat this problem. They obtain an equation for the eigenfunction of the total Hamiltonian by expanding this eigenfunction, insofar as it is a function of the coordinate of the electron of the hydrogen atom, in terms of the eigenfunctionsof the hydrogen Hamiltonian, having imposed suitable conditions on the coefficients of this expansion. In their treatment of exchange scattering they use this same eigenfunction of the total Hamiltonian, re-expand it, this time insofar as it is a function of the coordinate of the scattered electron, in terms of the eigenfunctions of the hydrogen Hamiltonian. Mott and Massy then assume certain conditions on the coefficient of the second expansion. It is our purpose to show in which sense their assumption is correct. We now proceed to discuss the assumption explicitly.

Let us denote by the subscript 1 the electron which is scattered and by the subscript 2 the electron of the hydrogen atom. Then the Hamiltonian for the problem is the following:

$$H(\underset{\sim}{x}_1,\underset{\sim}{x}_2) = T(\underset{\sim}{x}_1) + H_H(\underset{\sim}{x}_2) + V(\underset{\sim}{x}_1,\underset{\sim}{x}_2) + V(\underset{\sim}{x}_1). \qquad (1)$$

The operator $T(\underset{\sim}{x})$ is the kinetic-energy Hamiltonian for a particle of mass m:

$$T(\underset{\sim}{x}) = -\frac{1}{2m}\nabla^2. \qquad (2)$$

The operator $H_H(\underset{\sim}{x})$ is the hydrogenic Hamiltonian which we take as

$$H_H(\underset{\sim}{x}) = T(\underset{\sim}{x}) + V(\underset{\sim}{x}). \qquad (3)$$

$V(\underset{\sim}{x})$ is the interaction of an electron with the nucleus, and $V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ is the interaction of the two electrons with each other. These interactions take the place of the usual Coulomb interactions.

In the above expressions we have taken $\hbar = 1$ and have designated the three coordinates collectively of the first electron by the vector $\underset{\sim}{x}_1$ and those of the second electron by $\underset{\sim}{x}_2$.

We are interested in eigenfunctions of the total Hamiltonian $H(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ which describe a situation which corresponds to the condition that before collision the atom have the energy E_a and that the energy of the incident electron be $E - E_a$. We shall denote this eigenstate by $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a)$. The total energy initially is thus E. Since the energy of the system is a constant, the total energy of the system at any time is E also, so that $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a)$ is an eigenfunction of the total Hamiltonian $H(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ corresponding to the eigenvalue E; i.e.,

$$H(\underset{\sim}{x}_1,\underset{\sim}{x}_2)\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a) = E\psi(\underset{\sim}{x}_1\underset{\sim}{x}_2|E,E_a). \tag{4}$$

To specify the boundary conditions on $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a)$ corresponding to the initial condition, we introduce the eigenfunctions of $T(\underset{\sim}{x})$ and $H_H(\underset{\sim}{x})$.

Let us designate the eigenfunctions of $T(\underset{\sim}{x})$ associated with the energy E by $\chi(\underset{\sim}{x}|E)$; then

$$T(\underset{\sim}{x})\chi(\underset{\sim}{x}|E) = E\chi(\underset{\sim}{x}|E), \tag{5}$$

where E is in a continuum whose values range from 0 to $+\infty$. Furthermore, let us denote the eigenfunctions of $H_H(\underset{\sim}{x})$ associated with the energy E by $\phi(\underset{\sim}{x}|E)$. Thus

$$H_H(\underset{\sim}{x})\ \phi(\underset{\sim}{x}|E) = E\phi(\underset{\sim}{x}|E). \tag{6}$$

The argument E of $\phi(\underset{\sim}{x}|E)$ has discrete values for $E < 0$ and lies in the continuum for $0 < E < +\infty$. We shall call the lowest of the discrete eigenvalues

E_g (g indicates "ground" state).

Mott and Massey expand $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a)$ in terms of the eigenfunctions $\phi(\underset{\sim}{x}_2|E)$, as follows:

$$\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a) = \int_{E_g}^{\infty} F(\underset{\sim}{x}_1|E,E_a|E')\phi(\underset{\sim}{x}_2|E')dE', \qquad (7)$$

where the integration is to be understood as a summation over values of E' belonging to the discrete spectrum of H_H.

The functions $F(\underset{\sim}{x}_1|E,E_a|E')$ have the significance that $|F(\underset{\sim}{x}_1|E,E_a|E')^2$ is the probability density of finding electron 1 at $\underset{\sim}{x}_1$ when electron 2 is in the state $\phi(\underset{\sim}{x}_2|E')$ and when the entire system has the energy E. Mott and Massey prescribe that the asymptotic form of $F(\underset{\sim}{x}|E,E_a|E')$ shall be as follows when $|\underset{\sim}{x}_1| \rightarrow \infty$:

$$F(\underset{\sim}{x}_1|E,E_a|E') \rightarrow \delta(E'-E_a)\psi(\underset{\sim}{x}_1|E-E_a) + \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}_1|}}{|\underset{\sim}{x}_1|} f(\theta), \qquad (8)$$

where $\delta(E'-E_a)$ is to be taken as a Kronecker δ if both E' and E_a are in the discrete spectrum of H_H, as a Dirac δ if both are in the continuous spectrum of H_H, and as zero otherwise. Also

$$|\underset{\sim}{p}'| = \sqrt{2m(E-E')} \; . \qquad (9)$$

This boundary condition corresponds to the condition which we want, namely that before collision the atom be in the state of energy E_a and the incident particle have the kinetic energy $E-E_a$. After collision there is to be a flux of outgoing electrons.

Mott and Massey's conjecture is that if we use the expansion

$$\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a) = \int G(\underset{\sim}{x}_2|E,E_a|E')\ \phi(\underset{\sim}{x}_1|E')dE' \qquad (10)$$

instead of expansion (7), then $G(\underset{\sim}{x}_2|E,E_a|E')$ will behave like

$$\frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}_2|}}{|\underset{\sim}{x}_2|} g(\theta)$$

for $|\underset{\sim}{x}_2| \rightarrow \infty$. That is, haveing prescribed $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a)$ by imposing boundary condition (8) with respect to $\underset{\sim}{x}_1$, we assume that the outgoing wave condition on $\underset{\sim}{x}_2$ can be proved.

The significance of $G(\underset{\sim}{x}_2|E,E_a|E')$ is that $|G(\underset{\sim}{x}_2|E,E_a|E')|^2$ is the probability density that the second electron is at $\underset{\sim}{x}_2$ when the first electron has been captured by the hydrogen atom and is in the state $\phi(\underset{\sim}{x}_1|E')$. Since initially the first electron was free and the second electron was part of the hydrogen atom, whereas after collision $|G(\underset{\sim}{x}_2|E,E_a|E')|^2$ for $|\underset{\sim}{x}_1| \rightarrow \infty$ gives the probability that the first is part of the hydrogen atom and the second is free, $|G(\underset{\sim}{x}_2|E,E_a|E')|^2$ is called the "exchange probability".

In the following section we proceed to show in what sense Mott and Massey's conjecture is valid.

2. More Explicit Discussion of the Eigenfunctions

In order to prove the conjecture we must be more explicit as to the nature of the eigenfunctions involved. In particular, we shall have to take into account the auxilliary variables, which together with the Hamiltonian form a complete set of commuting variables. First let us consider the eigenfunctions of the kinetic energy operator $T(\underset{\sim}{x})$. Usually the three momentum components are taken as the complete set of commuting variables. For our purpose, however, we shall take as the complete set of commuting variables the energy and the polar angles of the momentum θ, ω. In terms of these variables we write the eigenfunctions of $T(\underset{\sim}{x})$ corresponding to the energy eigenvalue E as

$$\chi(\underset{\sim}{x}|E,\theta,\omega) = (2\pi)^{-3/2}(2m^3E)^{1/4}(\sin\theta)^{1/2}e^{i(\underset{\sim}{p}\,\underset{\sim}{x})}. \qquad (11)$$

Here $(\underset{\sim}{p}\underset{\sim}{x})$ is the inner product of the momentum vector $\underset{\sim}{p}$ and the coordinate vector $\underset{\sim}{x}$. In the right hand side of (11) we replace p_x, p_y, p_z by $\sqrt{2mE}\sin\theta\cos\omega$, $\sqrt{2mE}\sin\theta\sin\omega$, and $\sqrt{2mE}\cos\theta$ respectively. The eigenfunctions as chosen above satisfy the normalization conditions

$$\int \chi(\underset{\sim}{x}|E,\theta,\omega)\chi(\underset{\sim}{x}|E',\theta',\omega')d\underset{\sim}{x} = \delta(E-E')\delta(\theta-\theta')\delta(\omega-\omega')$$

$$\int_0^\infty\int_0^\pi\int_0^{2\pi}\chi(\underset{\sim}{x}|E,\theta,\omega)\,\chi(\underset{\sim}{x}'|E,\theta,\omega)d\omega d\theta dE = \delta(\underset{\sim}{x}-\underset{\sim}{x}'). \tag{12}$$

For simplicity we shall denote the angular variables θ, ω collectively by the variable α, so that the orthonormality conditions (12) become

$$\begin{aligned}&\int\chi(\underset{\sim}{x}|E,\alpha)\chi(\underset{\sim}{x}|E',\alpha')d\underset{\sim}{x} = \delta(E-E')\delta(\alpha,\alpha')\\ &\int_0^\infty\int\chi(\underset{\sim}{x}|E,\alpha)\chi(\underset{\sim}{x}'|E,\alpha)d\alpha dE = \delta(\underset{\sim}{x}-\underset{\sim}{x}'),\end{aligned} \tag{12a}$$

where we write

$$\chi(\underset{\sim}{x},|E,\alpha) \equiv \chi(\underset{\sim}{x}|E,\theta,\omega). \tag{13}$$

Let us now consider the eigenfunctions of $H_H(\underset{\sim}{x}) = T(\underset{\sim}{x}) + V(\underset{\sim}{x})$ and for the moment restrict ourselves to the continuous spectrum. If we assume that $V(\underset{\sim}{x})$ dies sufficiently rapidly, we may write the eigenfunctions of $H_H(\underset{\sim}{x})$ belonging to the continuous spectrum as the sum of an "incident wave" which is an eigenfunction of $T(\underset{\sim}{x})$ and a "scattered wave". We shall prescribe the boundary condition that the scattered wave shall be a radially outgoing wave. This condition is the one which will enable us to prove the conjecture. Mott and Massey are not explicit as to the nature of the eigenfunctions of H_H in the continuous spectrum. In the expansions (7) and (10) for F and G we shall have to use eigenfunctions of H_H with these boundary conditions.

Now as auxilliary variables we shall take the polar angles which describe the incident wave. The eigenfunctions of H_H belonging to the eigenvalue E for $E > 0$ satisfy the following integral equation:

$$\phi(\underset{\sim}{x}|E,\theta,\omega) = \chi(\underset{\sim}{x}|E,\theta,\omega) - \frac{m}{2\pi}\int \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x} - \underset{\sim}{x}'|} V(\underset{\sim}{x}')\phi(\underset{\sim}{x}'|E,\theta,\omega)d\underset{\sim}{x}', \qquad (14)$$

where $|\underset{\sim}{p}'| = \sqrt{2mE}$.

If, as before, we denote collectively the polar variables θ, ω by α we have

$$\phi(\underset{\sim}{x}|E,\alpha) = \chi(\underset{\sim}{x}|E,\alpha) - \frac{m}{2\pi}\int \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|} V(\underset{\sim}{x}')\phi(\underset{\sim}{x}'|E,\alpha)d\underset{\sim}{x}',$$

$$|\underset{\sim}{p}'| = \sqrt{2mE}\ . \qquad (14a)$$

For the discrete spectrum, i.e., for $E < 0$, we may choose any convenient set of auxilliary variables: for example, we might choose the total angular momentum if $V(\underset{\sim}{x})$ is spherically symmetric. Denoting these auxilliary variables by α, as above, but keeping in mind that α may be quantum numbers of an entirely different character than the α used for $E > 0$, we have as the integral equation for $E < 0$

$$\phi(\underset{\sim}{x}|E,\alpha) = - \frac{m}{2\pi}\int \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|} V(\underset{\sim}{x}')\phi(\underset{\sim}{x}'|E,\alpha)d\underset{\sim}{x}',$$

$$|\underset{\sim}{p}'| = \sqrt{2mE}\ . \qquad (15)$$

Note that since E is negative, $|\underset{\sim}{p}'|$ is imaginary and hence that $\phi(\underset{\sim}{x}|E,\alpha)$ decays exponentially for $|\underset{\sim}{x}| \to \infty$, as required. We can combine (14a) and (15) as follows:

$$\phi(\underset{\sim}{x}|E,\alpha) = \eta(E)\chi(\underset{\sim}{x}|E,\alpha) - \frac{m}{2\pi}\int \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|} V(\underset{\sim}{x}')\phi(\underset{\sim}{x}'|E,\alpha)d\underset{\sim}{x}',$$

$$|\underset{\sim}{p}'| = \sqrt{2mE}\ , \qquad (16)$$

where $\eta(E)$ is a step function given by

$$\begin{aligned} \eta(E) &= 1 \qquad E > 0 \\ \eta(E) &= 0 \qquad E < 0\ . \end{aligned} \qquad (17)$$

These functions satisfy the orthonormality relations

$$\begin{aligned}&\int \phi(\underset{\sim}{x}|E,\alpha)\,\phi(\underset{\sim}{x}|E',\alpha')\,d\underset{\sim}{x} = \delta(E-E')\delta(\alpha,\alpha')\\&\iint \phi(\underset{\sim}{x}|E,\alpha)\phi(\underset{\sim}{x}'|E,\alpha)d\alpha dE = \delta(\underset{\sim}{x}-\underset{\sim}{x}'),\end{aligned} \tag{18}$$

where one has to use care in interpreting $\delta(\alpha,\alpha')$ or equivalently the integration over α, since α may change character for $E > 0$ or $E < 0$. The $\delta(E-E')$ is to be interpreted as a Kronecker δ if the arguments belong to the discrete spectrum.

Our notational convention is the following:

Generally we shall denote eigenvalues of energy operators by capital Roman letters and eigenvalues corresponding to the auxilliary variables by small Greek letters. The range and nature of the eigenvalues are to be read off from the way in which they appear in the various eigenfunctions. We shall not hesitate to relabel the eigenvalues where necessary to prevent confusion, especially in integrations where they appear as dummy variables.

Now let us consider the eigenfunctions of the total Hamiltonian H which we previously denoted by $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a)$. We must now also indicate the dependence of the eigenfunction on the direction of the incident electron, which we shall call α_a, and on the initial auxilliary quantum number of the hydrogenic atom, which we call β_a. We shall now denote this eigenfunction by $\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)$. We write the expansion (7) as

$$\begin{aligned}&\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)\\&\quad = \int_{E_g}^{\infty}\int F(\underset{\sim}{x}_1|E,E_a,\alpha_a,\beta_a|E',\beta')\phi(\underset{\sim}{x}_2|E',\beta')d\beta' dE'.\end{aligned} \tag{19}$$

In (19) and everywhere below, integrations over variables which belong to the discrete spectrum are to be replaced by summations. We impose the condition that for $|\underset{\sim}{x}_1| \to \infty$, $F(x_1|E,E_a,\alpha_a,\beta_a|E',\beta')$ shall be the sum of an incident wave

$$\delta(E'-E_a)\delta(\beta-\beta_a)\,\chi(\underset{\sim}{x}_1|E-E_a,\alpha_a)$$

and a radially outgoing wave. Substituting (19) into (4) and using the orthonormality conditions on $\phi(\underset{\sim}{x}|E,\beta)$ one obtains the following integral equation for F which satisfies the boundary conditions:

$$F(\underset{\sim}{x}_1|E,E_a,\alpha_a,\beta_a|E',\beta') = \delta(E'-E_a)\delta(\beta'-\beta_a)\chi(\underset{\sim}{x}_1|E-E_a,\alpha_a)$$
$$-\frac{m}{2\pi}\iint \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}}{|\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}\left[\underline{V}(\underset{\sim}{x}_1')+V(\underset{\sim}{x}_1',\underset{\sim}{x}_2')\right]\phi(\underset{\sim}{x}_2'|E',\beta') \tag{20}$$
$$\cdot\,\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta')d\underset{\sim}{x}_1'd\underset{\sim}{x}_2'$$

with

$$|\underset{\sim}{p}'| = \sqrt{2m(E-E')}\quad ,$$

which, when substituted into (19), gives us the integral equation for ψ:

$$\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a) = \chi(\underset{\sim}{x}_1|E-E_a,\alpha_a)\;\phi(\underset{\sim}{x}_2|E_a,\beta_a)$$
$$-\frac{m}{2\pi}\int_{E_g}^{\infty}\iiint \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}}{|\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}\phi(\underset{\sim}{x}_2|E',\beta')\phi(\underset{\sim}{x}_2'|E',\beta') \tag{21}$$
$$\cdot\left[\underline{V}(\underset{\sim}{x}_1')+V(\underset{\sim}{x}_1',\underset{\sim}{x}_2')\right]\psi(\underset{\sim}{x}_1',\underset{\sim}{x}_2'|E,E_a,\alpha_a,\beta_a)d\underset{\sim}{x}_1'd\underset{\sim}{x}_2'd\beta'dE',$$

with

$$|\underset{\sim}{p}'| = \sqrt{2m(E-E')}\quad .$$

We shall discuss eigenfunctions of two more Hamiltonians which will be useful. The Hamiltonian H_o is defined by

$$H_o(\underset{\sim}{x}_1,\underset{\sim}{x}_2) = T(\underset{\sim}{x}_1) + H_H(\underset{\sim}{x}_2). \tag{22}$$

The incident term of the integral equation (21) is an eigenfunction of H_o corresponding to the eigenvalue E. We note that

$$H(\underset{\sim}{x}_1,\underset{\sim}{x}_2) = H_o(\underset{\sim}{x}_1,\underset{\sim}{x}_2) + V(\underset{\sim}{x}_1) + V(\underset{\sim}{x}_1,\underset{\sim}{x}_2); \tag{23}$$

hence (21) gives the eigenfunction of H in terms of a Green's function of

$(E-H_0)$, where $V(\underset{\sim}{x}_1) + V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ is considered a perturbation. We shall denote the eigenfunction of $H_0(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ corresponding to the eigenvalue E, by $\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta)$, where

$$\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta) = \chi(\underset{\sim}{x}_1|E-E',\alpha)\phi(\underset{\sim}{x}_2|E',\beta). \tag{24}$$

The eigenfunction $\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta)$ is an eigenfunction corresponding to the situation where the first electron is in the free state $\chi(\underset{\sim}{x}_1|E-E',\alpha)$ and the second is in the hydrogenic state $\phi(\underset{\sim}{x}_2|E',\beta)$. From the orthonormality conditions on ϕ and χ we have

$$\begin{gathered}\iint \bar{\lambda}(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta)\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|\bar{E},\bar{E}',\bar{\alpha},\bar{\beta})\,d\underset{\sim}{x}_1 d\underset{\sim}{x}_2 = \delta(E-\bar{E})\delta(E'-\bar{E}')\delta(\alpha-\bar{\alpha})\delta(\beta-\bar{\beta}), \\ \int_{E_g}^{\infty}\int_{E'}^{\infty}\iint \bar{\lambda}(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta)\lambda(\underset{\sim}{x}_1',\underset{\sim}{x}_2'|E,E',\alpha,\beta)\,d\alpha\,d\beta\,dE\,dE' = \delta(\underset{\sim}{x}_1-\underset{\sim}{x}_1')\delta(\underset{\sim}{x}_2-\underset{\sim}{x}_2').\end{gathered} \tag{25}$$

Integrations with respect to E have the limits from E' to +∞. Integrations with respect to E' range from E_g to ∞. Thus the order of integration is important: one must integrate over E first. The last Hamiltonian which we shall introduce is $H_1(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$, which is just $H_0(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ with the first and second particles interchanged:

$$H_1(\underset{\sim}{x}_1,\underset{\sim}{x}_2) = H_0(\underset{\sim}{x}_2,\underset{\sim}{x}_1). \tag{26}$$

The eigenfunctions of H_1 corresponding to the eigenvalue E are given by

$$\mu(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta) = \lambda(\underset{\sim}{x}_2,\underset{\sim}{x}_1|E,E',\alpha,\beta) = \chi(\underset{\sim}{x}_2|E-E',\alpha)\phi(\underset{\sim}{x}_1|E',\beta). \tag{27}$$

The eigenfunction $\mu(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E',\alpha,\beta)$ is the state vector corresponding to the first electron's being in the hydrogenic state $\phi(\underset{\sim}{x}_1|E',\beta)$ and the second electron's being the state $\chi(\underset{\sim}{x}_2|E-E',\alpha)$. The orthonormality relations for μ are analogous to those for λ.

3. Method of Proof

The function $G(\underset{\sim}{x}_2|E,E_a|E')$, which we now call $G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta')$, is defined by the alternative expansion (10), which we now write as

$$\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a) = \int_{E_g}^{\infty}\int G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta')\phi(\underset{\sim}{x}_1|E',\beta')d\beta' dE' \; . \tag{28}$$

Using the orthogonality relations (18) for ϕ we have

$$G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta') = \int \psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)\bar{\phi}(\underset{\sim}{x}_1|E',\beta')d\underset{\sim}{x} \; . \tag{29}$$

To show that G is an outgoing spherical wave in $\underset{\sim}{x}_2$ we shall use the integral equations (21) for ψ. However, to isolate the outgoing part, it is convenient to work in the H_1 representation since the outgoing part will be recognizable in this representation as a δ_+ —function.

Let us denote ψ in the H_1 representation by $r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a)$, which is given by

$$r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) = \iint \psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a) \cdot \mu(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,G,\gamma,\epsilon)d\underset{\sim}{x}_1 d\underset{\sim}{x}_2, \tag{30}$$

μ being the eigenfunction of H_2. Using the orthogonality relations (18), (12) for ϕ and χ and the expression (27) for μ, we see that (29) is equivalent to

$$G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|F',\beta') = \int_{E'}^{\infty}\int r(F,E',\gamma,\beta'|E,E_a,\alpha_a,\beta_a)\chi(x_2|F-E',\gamma)d\gamma dF. \tag{31}$$

We shall calculate r in terms of ψ as given in the H_o—representation.

Denoting ψ in the H_0 by $u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a)$, where

$$u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) = \iint \psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,G,\gamma,\epsilon)d\underset{\sim}{x}_1 d\underset{\sim}{x}_2, \qquad (32)$$

we have, on using (30), (27) and (25) together with orthogonality relations for ϕ and χ :

$$r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) = \int_{E_g}^{\infty}\int_{G'}^{\infty}\iint u(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a)$$

$$\cdot\, v(F-G,\gamma|G',\epsilon')\,\bar{v}(F'-G',\gamma'|G,\epsilon)d\gamma' d\epsilon' dF' d,G \qquad (33)$$

where

$$v(E,\alpha|F,\beta) = \int \bar{\chi}\,(\underset{\sim}{x}|E,\alpha)\phi(\underset{\sim}{x}|F,\beta)d\underset{\sim}{x}\ ; \qquad (34)$$

$v(E,\alpha|F,\beta)$ is thus the eigenfunction ϕ of H_H as given in the representation of the kinetic energy operator T. We shall use the integral equations for u and v to obtain the outgoing parts and finally use (33) and (31) to get the expression for G.

4. The Equations for u and v

We shall first show that $u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a)$ satisfies the relation

$$u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) = \delta(F-E)\delta(G-E_a)\delta(\gamma-\alpha_a)\delta(\epsilon-\beta_a)$$

$$+\ \gamma_-(E-F)T(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a), \qquad (35)$$

where

$$T(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a)$$

$$= \iint \bar{\chi}\,(\underset{\sim}{x}_1|F-G,\gamma)\phi(\underset{\sim}{x}_2|G,\epsilon)\ [\bar{V}(\underset{\sim}{x}_1) + V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)] \qquad (36)$$

$$\cdot\ \psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)\ d\underset{\sim}{x}_1\ d\underset{\sim}{x}_2$$

and where $\gamma_-(\zeta)$ is essentially the δ_+ function; it is defined by

$$\gamma_-(\zeta) = \lim_{\xi \to +0} \frac{1}{\zeta + i\xi} = -i\pi\delta(\zeta) + P\frac{1}{\zeta}, \tag{37}$$

where P indicates that in integrations over ζ, the principal part of the integral is to be used. It might be noted that in accordance with the general formalism of scattering operators, $T(E,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a)$ is the amplitude of the scattered spherical wave obtained when one sets $|\underset{\smile}{x}_1| \to \infty$ in the integral equation for ψ (eqn.(21)). This scattered wave corresponds to the case where after scattering the hydrogen atom is in the state described by the quantum numbers G, γ.

Incidentally, one can write (35) as an integral equation for u, namely

$$\begin{aligned} u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) &= \delta(F-E)\delta(G-E_a)\delta(\gamma-\alpha_a)\delta(\epsilon-\beta_a) \\ &+ \gamma_-(E-F)\left[V(x_1)+V(\underset{\smile}{x}_1,\underset{\sim}{x}_2)\right]^{H_o} u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) \end{aligned} \tag{35a}$$

where $\left[V(\underset{\sim}{x}_1)+V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)\right]^{H_o}$ is the operator $V(\underset{\sim}{x}_1)+V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ as given in the H_o representation; it operates on the variables F,G,γ,ϵ of

$$u(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a)$$

on the right hand side of (35a). Equation (35a) can be made the basis of a discussion of the scattering problem in terms of the scattering operator (see e.g. Moses, ref. [2]).

The proof of (35) involves the following well-known identity:

$$\begin{aligned} &\int_0^\infty \int_0^\pi \int_0^{2\pi} \bar{\chi}(\underset{\smile}{x}|E,\theta,\omega)\gamma_-(F-E)\chi(\underset{\sim}{x}'|E,\theta,\omega)\,d\omega\, d\theta\, dE \\ &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \bar{\chi}(\underset{\smile}{x}'|E,\theta,\omega)\gamma_-(F-E)\chi(x|E,\theta,\omega)\,d\omega\, d\theta\, dE = -\frac{m}{2\pi}\,\frac{e^{i|p||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\smile}{x}-\underset{\sim}{x}'|} \end{aligned} \tag{38}$$

where

$$|\underset{\smile}{p}| = \sqrt{2mF}\,.$$

The verification of (35) is obtained by replacing ψ in equation (32) by the righthand side of (21). Using the identity (38) we replace

$$-\frac{m}{2\pi}\,\frac{e^{i|p'||\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}}{|\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}\,,\ \text{with } |p'| = \sqrt{2m}\,(E-E'),$$

by

$$\int_0^\infty\int\bar{\chi}(\underset{\sim}{x}_1'|F',\alpha')\,\gamma_-(E-E'-F')\,\chi(\underset{\sim}{x}_1|F',\alpha')\,d\alpha'\,dF'$$

$$=\int_{E'}^\infty\int\bar{\chi}(\underset{\sim}{x}_1'|F'-E',\alpha')\,\gamma_-(E-F')\,\chi(\underset{\sim}{x}_1|F'-E',\alpha')\,d\alpha'\,dF'.$$

We then have

$$u(F,G,\nu,\epsilon|E,E_a,\alpha_a,\beta_a) = \iint\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,G,\nu,\epsilon)\,d\underset{\sim}{x}_1\,d\underset{\sim}{x}_2$$

$$+\int d\underset{\sim}{x}_1'\int d\underset{\sim}{x}_2'\int_{E_g}^\infty dE'\int_{E'}^\infty dF'\int d\beta'\int d\alpha'\,\bar{\chi}(\underset{\sim}{x}_1'|F'-E',\alpha')\phi(\underset{\sim}{x}_2'|E',\beta)$$

$$\cdot\,\gamma_-(E-F')\left[\bar{V}(\underset{\sim}{x}_1')+V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)\right]\psi(\underset{\sim}{x}_1',\underset{\sim}{x}_2'|E,E_a,\alpha_a,\beta_a)$$

$$\cdot\left[\int d\underset{\sim}{x}_1\,\chi(\underset{\sim}{x}_1|F'-E',\alpha')\bar{\chi}(\underset{\sim}{x}_1|F-G,\gamma)\right]$$

$$\cdot\left[\int d\underset{\sim}{x}_2\,\phi(\underset{\sim}{x}_2|E',\beta')\phi(\underset{\sim}{x}_2|G,\epsilon)\right]\quad,$$

which, on using the orthonormality conditions on ϕ, χ, λ, gives (35).

Similarly we find for v

$$v(E,\alpha|F,\beta) = \eta(F)\delta(E-F)\delta(\alpha-\beta)+\gamma_-(F-E)T_1(E,\alpha|F,\beta), \qquad (39)$$

where

$$T_1(E,\alpha|F,\beta) = \int\bar{\chi}(\underset{\sim}{x}|E,\alpha)V(\underset{\sim}{x})\phi(\underset{\sim}{x}|F,\beta)\,d\underset{\sim}{x}\ . \qquad (40)$$

5. The Evaluation of $r(F,G,\nu,\epsilon|E,E_a,\alpha_a,\beta_a)$.

We shall obtain r in several steps; in each step it will be our objective to isolate a γ_- function, since this function in the $\underset{\sim}{x}$ representation is the radially outgoing wave. We shall first indicate several useful identities for γ_-. First, from (37) we have

$$\bar{\gamma}_-(\zeta) = -\gamma_-(-\zeta). \tag{41}$$

It can also be shown that

$$\gamma_-(\zeta_1)\,\gamma_-(\zeta_2) = \gamma_-(\zeta_1)\gamma_-(\zeta_1+\zeta_2) + \gamma_-(\zeta_2)\,\gamma_-(\zeta_1+\zeta_2)\,. \tag{42}$$

On using (41) we see that (42) can be written as

$$\bar{\gamma}_-(\zeta_1)\,\gamma_-(\zeta_2) = \bar{\gamma}_-(\zeta_1)\gamma_-(\zeta_2-\zeta_1) + \gamma_-(\zeta_2)\,\bar{\gamma}_-(\zeta_1-\zeta_2). \tag{43}$$

In expression (33) we note that the product $v(F-G,\gamma|G',\epsilon')\bar{v}(F'-G',\gamma'|G,\epsilon)$ appears. We shall use the identity (43) and equation (39) for v to isolate a γ_- function.

From (39) we obtain immediately

$$\begin{aligned} v(E,\alpha|F,\beta)\,\bar{v}(E',\alpha'|F',\beta') &= \eta(F)\,\eta(F')\delta(E-F)\delta(E'-F')\delta(\alpha-\beta)\delta(\alpha'-\beta') \\ &\quad + \eta(F)\delta(E-F)\delta(\alpha-\beta)\bar{\gamma}_-(F'-E')\bar{T}_1(E',\alpha'|F',\beta') \\ &\quad + \eta(F')\delta(E'-F')\delta(\alpha'-\beta')\gamma_-(F-E)T_1(E,\alpha|F,\beta) \\ &\quad + \bar{\gamma}_-(F'-E')\gamma_-(F-E)T_1(E,\alpha|F,\beta)\bar{T}_1(E',\alpha'|F',\beta'). \end{aligned} \tag{44}$$

We shall simplify the last term of (44). Using (43) we have

$$\begin{aligned} &\bar{\gamma}_-(F'-E')\gamma_-(F-E) \\ &= \bar{\gamma}_-(F'-E')\gamma_-(F-E-F'+E')+\gamma_-(F-E)\bar{\gamma}_-(F'-E'-F+E). \end{aligned} \tag{45}$$

Hence the last term of (44) is

$$\begin{aligned} &\bar{\gamma}_-(F'-E')\bar{T}_1(E',\alpha'|F',\beta')\gamma_-(F-E-F'+E')T_1(E,\alpha|F,\beta) \\ &\qquad + \gamma_-(F-E)T_1(E,\alpha|F,\beta)\bar{\gamma}_-(F'-E'-F+E)\bar{T}_1(E',\alpha'|F',\beta') \\ &= \bar{v}(E',\alpha'|F',\beta')\gamma_-(F-E-F'+E')T_1(E,\alpha|F,\beta) \\ &\qquad - \eta(F')\delta(E'-F')\delta(\alpha'-\beta')\gamma_-(F-E-F'+E')T_1(E,\alpha|F,\beta) \\ &\quad + v(E,\alpha|F,\beta)\bar{\gamma}_-(F'-E'-F+E)\bar{T}_1(E',\alpha'|F',\beta') \\ &\qquad - \eta(F)\delta(E-F)\delta(\alpha-\beta)\bar{\gamma}_-(F'-E'-F+E)\bar{T}_1(E',\alpha'|F',\beta'), \end{aligned} \tag{46}$$

where we have used (39) to obtain $\gamma_- T_-$ in terms of v. Now the second and fourth terms on the right-hand side of (46) are just the negatives of the third and fourth terms on the right-hand side of equation (44). Hence, substituting the last term of (44) as given by (46), we have

$$
\begin{aligned}
&v(E,\alpha|F,\beta)\,\bar{v}(E',\alpha'|F',\beta') = \\
&\eta(F)\,\eta(F')\delta(E-F)\delta(E'-F')\delta(\alpha-\beta)\delta(\alpha'-\beta') \\
&+ \gamma_-(F-E-F'+E')\,\big[\bar{v}(E',\alpha'|F',\beta')T_1(E,\alpha|F,\beta) \\
&\qquad - v(E,\alpha|F,\beta)\bar{T}_1(E',\alpha'|F',\beta')\big],
\end{aligned}
\tag{47}
$$

from which we obtain finally

$$
\begin{aligned}
&v(F-G,\gamma|G',\epsilon')\,\bar{v}(F'-G',\gamma'|G,\epsilon) \\
&= \eta(G')\,\eta(G)\delta(F-F')\delta(F-G-G')\delta(\gamma-\epsilon')\delta(\gamma'-\epsilon) \\
&\quad + \gamma_-(F'-F)\,\big[\bar{v}(F'-G',\gamma'|G,\epsilon)T_1(F-G,\gamma|G',\epsilon') \\
&\qquad - v(F-G,\gamma|G',\epsilon')\bar{T}_1(F'-G',\gamma'|G,\epsilon)\big] .
\end{aligned}
\tag{48}
$$

In (48) we have achieved our aim of isolating a γ_- function.

To evaluate

$$
\begin{aligned}
&r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) \\
&= \int_{E_g}^{\infty}\int_{G'}^{\infty}\iint u(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a) \\
&\qquad \cdot v(F-G,\gamma|G',\epsilon')\,\bar{v}(F'-G',\gamma'|G,\epsilon)\,d\gamma' d\epsilon' dF' dG',
\end{aligned}
$$

we use expression (48) for the product of $v\,\bar{v}$, and for u we use equation (35). We obtain four terms as we did when we evaluated the product $v\,\bar{v}$. It turns out that by using (42) for the products of the γ_-'s of the fourth term one can eliminate two of the terms in a manner analogous to the derivation of (47). We have finally

$$
\begin{aligned}
r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) &= \eta(G)\eta(E_a)\delta(F-E)\delta(F-G-E_a)\delta(\epsilon-\alpha_a)\delta(\gamma-\beta_a) \\
&+ \nu_-(E-F)\Bigg\{\int_{E_g}^{\infty}\int_{G'}^{\infty}\iint v(F-G,\gamma|G',\epsilon')\bar{v}(F'-G',\gamma'|G,\epsilon)T(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a) \\
&\qquad \cdot d\gamma' d\epsilon' dF' dG' \\
&+ \int_{E_g}^{\infty}\int_{G'}^{\infty}\iint \bar{v}(F'-G',\gamma'|G,\epsilon)T_1(F-G,\gamma|G',\epsilon')u(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a)d\gamma' d\epsilon' dF' dG' \\
&- \int_{E_g}^{\infty}\int_{G'}^{\infty}\iint v(F-G,\gamma|G',\epsilon')\bar{T}_1(F'-G',\gamma'|G,\epsilon)u(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a)d\gamma' d\epsilon' dF' dG' \Bigg\}.
\end{aligned}
\tag{49}
$$

Now, using the definition (34), (40), (32), (36) for v, T_1 and u,T respectively, and the orthonormality properties for χ and ϕ, one obtains

$$
\begin{aligned}
&\int_{E_g}^{\infty}\int_{G'}^{\infty}\iint v(F-G,\gamma|G',\epsilon')\bar{v}(F'-G',\gamma'|G,\epsilon)T(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a)d\gamma' d\epsilon' dF' dG' \\
&= \iint \bar{\chi}(\underset{\sim}{x}_2|F-G,\gamma)\phi(\underset{\sim}{x}_1|G,\epsilon)\,[V(\underset{\sim}{x}_1) + V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)]\,\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)d\underset{\sim}{x}_1 d\underset{\sim}{x}_2\,,
\end{aligned}
\tag{50}
$$

$$
\begin{aligned}
&\int_{E_g}^{\infty}\int_{G'}^{\infty}\iint \bar{v}(F'-G',\gamma'|G,\epsilon)T_1(F-G,\gamma|G',\epsilon')u(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a)d\gamma' d\epsilon' dF' dG' \\
&= \iint \bar{\chi}(\underset{\sim}{x}_2|F-G,\gamma)\phi(\underset{\sim}{x}_1|G,\epsilon)V(\underset{\sim}{x}_2)\,\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)d\underset{\sim}{x}_1 d\underset{\sim}{x}_2\,,
\end{aligned}
\tag{51}
$$

and

$$
\begin{aligned}
&\int_{E_g}^{\infty}\int_{G'}^{\infty}\iint v(F-G,\gamma|G',\epsilon')\bar{T}_1(F'-G',\gamma'|G,\epsilon)u(F',G',\gamma',\epsilon'|E,E_a,\alpha_a,\beta_a)d\gamma' d\epsilon' dF' dG' \\
&= \iint \bar{\chi}(\underset{\sim}{x}_2|F-G,\gamma)\bar{\phi}(\underset{\sim}{x}_1|G,\epsilon)V(\underset{\sim}{x}_1)\,\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)d\underset{\sim}{x}_1 d\underset{\sim}{x}_2.
\end{aligned}
\tag{52}
$$

Hence we have finally

$$
\begin{aligned}
r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) &= \eta(G)\eta(E_a)\delta(F-E)\delta(F-G-E_a)\delta(\epsilon-\alpha_a)\delta(\gamma-\beta_a) \\
&+ \gamma_-(E-F)\iint \bar{\chi}(\underset{\sim}{x}_2|F-G,\gamma)\bar{\phi}(\underset{\sim}{x}_1|G,\epsilon) \\
&\cdot [V(\underset{\sim}{x}_1,\underset{\sim}{x}_2) + V(\underset{\sim}{x}_2)]\,\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)d\underset{\sim}{x}_1 d\underset{\sim}{x}_2\,.
\end{aligned}
\tag{53}
$$

Equation (53) can be written as an integral equation for

$$r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a),$$

as follows:

$$r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) = \eta(G)\eta(E_a)\delta(F-E)\delta(F-G-E_a)\delta(\epsilon-\alpha_a)\delta(\gamma-\beta_a)$$
$$+ \gamma_-(E-F)\ \left[V(\underset{\sim}{x}_1,\underset{\sim}{x}_2) + V(\underset{\sim}{x}_2)\right]^{H_1} r(F,G,\gamma,\epsilon|E,E_a,\alpha_a,\beta_a) \tag{53a}$$

where $\left[V(\underset{\sim}{x}_1,\underset{\sim}{x}_2) + V(\underset{\sim}{x}_2)\right]^{H_1}$ is the operator $V(\underset{\sim}{x}_1,\underset{\sim}{x}_2) + V(\underset{\sim}{x}_2)$ as given in the H_1 representation; it operates on the F, G, γ, ϵ variables of r on the right-hand side of (53a). Equations (21), (35a) and (53a) are the integral equations for the same eigenfunction of H in the $\underset{\sim}{x}$, H_o,H_1, - representations respectively.

6. The Evaluation of $G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta')$

Using equation (31) which gives G in terms of r, we have

$$G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta') = \eta(E')\ \eta(E_a)\ \chi(\underset{\sim}{x}_2|E-E',\beta_a)\delta(E-E'-E_a)\delta(\alpha_a-\beta')$$
$$+ \iint \left[\int_{E'}^{\infty}\!\!\int \chi(\underset{\sim}{x}_2|F-E',\gamma)\gamma_-(E-F)\,\overline{\chi}(\underset{\sim}{x}_2'|F-E',\gamma)d\gamma dF\right]$$
$$\cdot\ \overline{\phi}(\underset{\sim}{x}_1'|E',\beta')\ \left[V(\underset{\sim}{x}_1',\underset{\sim}{x}_2')+V(\underset{\sim}{x}_2')\right]\ \psi(\underset{\sim}{x}_1',\underset{\sim}{x}_2'|E,E_a,\alpha_a,\beta_a)d\underset{\sim}{x}_1'd\underset{\sim}{x}_2'\ .$$

Now we use (38) to obtain

$$\int_{E'}^{\infty}\!\!\int \chi(\underset{\sim}{x}_2|F-E',\gamma)\gamma_-(E-F)\,\overline{\chi}(\underset{\sim}{x}_2'|F-E',\gamma)d\gamma dF$$
$$= \int_{0}^{\infty}\!\!\int \chi(\underset{\sim}{x}_2|F,\gamma)\gamma_-(E-E'-F)\,\overline{\chi}(\underset{\sim}{x}_2'|F,\gamma)d\gamma dF \tag{54}$$
$$= -\frac{m}{2\pi}\ \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}_2-\underset{\sim}{x}_2'|}}{|\underset{\sim}{x}_2-\underset{\sim}{x}_2'|}\ ,$$

where

$$|\underset{\sim}{p}'| = \sqrt{2m(E-E')} \,.$$

Finally, our generalization of Mott and Massey's conjecture is

$$G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_e|E',\beta') = \eta(E')\eta(E_a)\chi(\underset{\sim}{x}_2|E_a,\beta_e)\delta(E-E'-E_a)\delta(\alpha_a-\beta') \tag{55}$$

$$-\frac{m}{2\pi}\iint \frac{e^{i|\underset{\sim}{p}'||\underset{\sim}{x}_2-\underset{\sim}{x}_2'|}}{|\underset{\sim}{x}_2-\underset{\sim}{x}_2'|}\,\overline{\phi}(\underset{\sim}{x}_1'|E',\beta')\left[V(\underset{\sim}{x}_1',\underset{\sim}{x}_2') + V(\underset{\sim}{x}_2')\right]\psi(\underset{\sim}{x}_1',\underset{\sim}{x}_2'|E,E_a,\alpha_a,\beta_a)\,d\underset{\sim}{x}_1'\,d\underset{\sim}{x}_2' \,,$$

where

$$|\underset{\sim}{p}'| = \sqrt{2m(E-E')}.$$

It is clear that the second term represents outgoing spherical waves. In Mott and Massey's conjecture the first term is ignored. If the initial state of the hydrogen atom is such that the electron is bound, then $E_a < 0$ and hence the first term vanishes for all E', β'. Even if initially the hydrogen atom is in an ionized state, the first term vanishes for $E' < 0$, i.e., for exchange scattering where the incident electron is captured.

Borowitz and Friedman [ref. 3] point out that the integral of the second term diverges for $E' > 0$. This is not surprising because G is a symbolic function in the sense of L. Schwartz. That is, G contains a part resembling δ-function. This is clear from the fact that the first term contains a δ-function. This statement can also be shown to be true on more fundamental grounds which we shall not discuss here.

Borowitz and Friedman extract the symbolic part of this integral and are left with a convergent part. We prefer to consider a wave packet of incident electrons and hydrogenic atoms as being given initially. The initial state would then be

$$\int_{E_e}^{\infty}\int_{E_a}^{\infty}\iint \lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)f(E,E_a,\alpha_a,\beta_a)\,d\alpha_a\,d\beta_a\,dE\,dE_a,$$

while at any finite time the state is given by

$$\int_{E_g}^{\infty}\int_{E_a}^{\infty}\iint \psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)f(E,E_a,\sigma_a,\beta_a)d\sigma_a d\beta_a dE dE_a,$$

where we take $f(E,E_a,\alpha_a,\beta_a)$ to be a quadrically integrable function of its arguments.

Then

$$\int_{E_g}^{\infty}\int_{E_a}^{\infty}\iint G(\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a|E',\beta')\ f(E,E_a,\alpha_a,\beta_a)d\alpha_a d\beta_a dE dE_a$$

is a well-defined function of $\underset{\sim}{x}_2$ and is the probability amplitude for exchange scattering.

Some generalizations of the above expressions are possible, for although we have assumed that $V(\underset{\sim}{x})$, $V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ are simply functions of their arguments, our results can be generalized to take into account the possibility that $V(\underset{\sim}{x})$, $V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)$ are operators. The generalization can be obtained immediately, but we refrain from giving it here explicitly.

It should be pointed out that the Mott and Massey's $F_n(\underset{\sim}{r})$, $G_n(\underset{\sim}{r})$, $\psi(\underset{\sim}{r}_1,\underset{\sim}{r}_2)$ are not quite our functions F, G, and ψ. They are related as follows:

$$F_n(\underset{\sim}{r}) = (2\pi)^{3/2}[2m^3(E-E_a)]^{-1/4}\sin^{-1/2}\theta_a F(\underset{\sim}{x}|E,E_a,\alpha_a,\beta_a|E',\beta')$$

$$\psi(\underset{\sim}{r}_1,\underset{\sim}{r}_2) = (2\pi)^{3/2}[2m^3(E-E_a)]^{-1/4}\sin^{-1/2}\theta_a\psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,E_a,\alpha_a,\beta_a)$$

$$G_n(\underset{\sim}{r}) = (2\pi)^{3/2}[2m^3(E-E_a)]^{-1/4}\sin^{-1/2}\theta_a G(\underset{\sim}{x}|E,E_a,\alpha_a,\beta_a|E',\beta')\ ,$$

where the quantum number n corresponds to the pair of quantum numbers E', β', and α_a represents the pair of polar angles θ_a, ω_a of the incident electron. Also, the vector $\underset{\sim}{r}$ is just our vector, $\underset{\sim}{x}$.

References

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